Saturday, June 21

08:45 Opening

Session 1

Chair: Abril Castro

09:00 Stefan Gugler [426]
Finding molecular minima and transition-states with reverse diffusion

09:20 Miguel Steiner [512]
Differentiable simulations for insight into multi-phase reaction mechanisms

09:40 Laura Grazioli [116]
Excited states as critical points of the potential energy surface

10:00 Nina Glaser [639]
Targeting Excited States on Early Fault Tolerant Quantum Computers

10:20 Frank Hu [519]
Accurate and efficient structure elucidation from NMR using artificial intelligence

10:40 - 11:10 break

Session 2

Chair: Thomas Bondo Pedersen

11:10 Fabian Faulstich [176]
A static quantum embedding scheme based on coupled cluster theory

11:30 Marti Gimferrer [756]
On the impact of nuclear quantum effects in intermolecular interactions

11:50 Ji Woong Yu [642]
Investigation of anomalous water dynamics using machine learning force field

12:10 Madhubanti Mukherjee [568]
Exploring Additives for Crystallization of Halide Perovskites in Solar Cells

12:30 - 14:10 break

Session 3

Chair: Michele Cascella

14:10 Marcos Casanova-Páez [410]
Core-Excited States for Open-Shell Systems in Similarity-Transformed Equation-of-Motion Theory

14:30 Torsha Moitra [556]
Real-time methods for light-induced attosecond spectroscopies

14:50 Ben McLean [275]
Thermodynamics of graft copolymer self-assembly in mixed solvents: Molecular dynamics

15:10 Róża Okoń [445]
Small-molecule energy carriers for prebiotic metabolism models

15:30 Mariia Ivonina [325]
Decoding SARS-CoV-2 Pseudoknot Dynamics: Unraveling Drug Interaction Mechanism

15:50 - 16:20 break

Session 4

Chair: Ainara Nova

16:20 Rebecca Tomann [750]
Efficient Extended Tight Binding Implementation with Linear Scaling Algorithms

16:40 Leonardo Dos Anjos Cunha [741]
Photonic observables and QEDFT functionals for strongly coupled light-matter systems

17:00 Sergio Moles Quintero [484]
Exploring Excited-State Aromaticity and Diradical Nature on Singlet Fission

17:20 Enric Petrus [694]
Automated Exploration of Ozonation Reactions for Model Olefins in Water

17:40 Closing

17:50 - 19:30 break

19:30 Young WATOC dinner (at Skullerud stua)

Sunday, June 22

15:00 Opening

Plenary P1

Chair: Odile Eisenstein

15:40 Michele Parrinello [927]
The weird and wonderful world of catalysis

16:20 Veronique van Speybroeck [829]
Is simpler better? Alternative wave function approaches for molecular modeling

17:00 - 17:30 break

Plenary P2

Chair: Peter Gill

17:30 Frank Neese [929]
The Bubblepole approximation for large molecular systems

18:10 Jan Martin [954]
Accurate thermochemistry, kinetics, and spectroscopy: the high and low roads

18:50 - 19:20 break

19:20 - 20:00 Mingling with refreshments

Monday, June 23

	Session A1	Session B1	Session C1	Session D1	Session E1
	CATALYSIS & REACTIVITY Reactants, reactions, and catalysis	ELECTRONIC-STRUCTURE THEORY Green's function methods	BIOSYSTEMS Cheminformatics & medicinal chemistry	COMPUTING & SOFTWARE Quantum computing	CHEMICAL STRUCTURE & BONDING Conjugated systems
	Chair: Kevin Naidoo	Chair: Andreas Görling	Chair: Stacey Wetmore	Chair: Ivan Kassal	Chair: Peter Schreiner
08:30	Raghavan Sunoj [963] *Computational Chemistry and Machine Learning Approaches in Asymmetric Catalysis*	Dominika Zgid [924] *Fully self-consistent finite temperature GW for correlated systems*	Jean-Louis Reymond [986] *Chemical Space from First Principles*	Birgitta Whaley [919] *Finding Quantum Advantage for Quantum Chemistry*	Debashree Ghosh [871] *Structure and photophysics of melanin*
08:55	Stuart Macgregor [926] *Modelling Ruthenium-Catalyzed N-Directed C–H Functionalization*	Wim Klopper [458] *Bethe-Salpeter Equation for Calculations of X-Ray Spectra*	Jan Řezáč [480] *PM6-ML: Synergy of Semiempirical Quantum Chemistry and Machine Learning*	Artur Izmaylov [131] *Optimizing Quantum Algorithms for Next-Generation Quantum Chemistry*	Abhik Ghosh [973] *Ground- and excited-state charge flow phenomena in metallocorroles*
09:20	Ashique Lal [207] *Unraveling CO2 Reduction with DFT Molecular Dynamics at Interfaces*	Marios-Petros Kitsaras [124] *Analytic Bethe-Salpeter equation excited-state gradients*	Elfi Kraka [130] *Revolutionizing Drug Discovery with SmartCADD: AI Meets Quantum Chemical Precision*	Davide Castaldo [327] *Accelerating quantum chemistry simulations on quantum computers with signal processing*	Martin Rahm [23] *Superconducting Radical Pancakes*
09:35	Boris Maryasin [127] *In Silico Organic Chemistry: From Small to Large Molecular Scales*	Arno Förster [572] *Consistent merging of GW and T-matrix self-energies*	Jean-Philip Piquemal [699] *A Foundation Model for Accurate Simulations in Drug Design*	Karl Michael Ziems [260] *Simulation of spectroscopic properties on quantum computers*	Takafumi Shiraogawa [313] *Antisymmetry rules of response properties in certain chemical spaces*
09:50	- 10:20	break			

Monday, June 23

	Session A2	Session B2	Session C2	Session D2	Session E2
	MACHINE LEARNING ML for simulations	CATALYSIS & REACTIVITY Surfaces and heterogenous catalysis	ELECTRONIC-STRUCTURE THEORY Numerical methods and techniques	BIOSYSTEMS Macromolecules	ELECTRONIC-STRUCTURE THEORY Ultrahigh accuracy and QED
	Chair: Heather Kulik	Chair: Angel Martín Pendás	Chair: Stefan Grimme	Chair: Benedetta Mennucci	Chair: Fritz Schaefer
10:20	Gábor Csányi [967] *Machine learning force fields shows extreme generalisation*	Philippe Sautet [873] *Can photocatalysis be sustained in the dark? A modeling perspective*	Peter Gill [953] *A New Approach to Density Functional Quadrature*	Lynn Kamerlin [49] *Loop Dynamics and the Origins of New Proteins*	Trond Saue [349] *Towards Highly Accurate Calculations of Molecular Properties*
10:45	Alexandre Tkatchenko [995] *Beyond AlphaFold and Empirical Potentials: Next-Generation Molecular Simulations with Machine-Learned Force Fields*	Núria López [972] *Simulations in complex environments from DFT to Machine Learning*	Luca Frediani [896] *Quantum Chemistry with Multiwavelets: from exotic niche to widespread applicability*	Subha Kalyaanamoorthy [653] *From Atoms to AI: Computational Design of Enzymes and Therapeutics*	Jacek Komasa [178] *Nonadiabatic relativistic and QED energy levels of the hydrogen molecule*
11:10	Jelle Vekeman [785] *Machine Learning Potentials at Speeds Comparable to Reactive Force Fields*	Christopher Stein [287] *Simple Embedding Models for Metallic Surfaces*	David Sherrill [513] *Symmetry-Adapted Perturbation Theory for Large Systems with Electrostatic Embedding*	Xiang Sheng [196] *Computational Modeling and Rational Design of Enzymes*	Ádám Margócsy [775] *Ultra-precise rovibrational intervals for the excited helium dimer*
11:25	Michael Gillhofer [317] *Buffer Region embedding for MLP/MM simulations in complex environments*	Mireia Segado-Centellas [716] *Water as Solvent and Reactant: Molecular Interactions and Electrokinetics*	Eduard Matito [136] *Modern Density Functional Approximations are Ill-designed to Compute Vibrational Properties*	Adil Kabylda [547] *(Bio)molecular Simulations with Pretrained Neural Network and Pairwise Force Fields*	Pekka Pyykkö [486] *Is relativistic quantum chemistry a good theory of everything?*
11:40	- 13:20	break			

Monday, June 23

	Session A3	Session B3	Session C3	Session D3	Session E3
	ELECTRONIC-STRUCTURE THEORY	ENERGY & MATERIALS	CATALYSIS & REACTIVITY	QUANTUM DYNAMICS	BIOSYSTEMS
	Coupled-cluster theory	Condensed systems	Molecular and reaction design	Nonadiabatic dynamics	Macromolecules
	Chair: Jürgen Gauss	Chair: Yi Qin Gao	Chair: Vidar Remi Jensen	Chair: Ove Christiansen	Chair: Elfi Kraka
13:20	Piotr Piecuch [923] *Recent Advances in the CC(P;Q) Methodology: CIPSI-Driven and Adaptive Approaches*	Francesco Paesani [752] *Predictive Data-Driven Many-Body Simulations of Water Across Phases and Environments*	Yousung Jung [441] *Predicting Organic Reactions Based on Electron Movements using Machine Learning*	Alicia Palacios [804] *Correlated electron and nuclear dynamics at the attosecond time scale*	Ferran Feixas [622] *Navigating the Conformational Landscape of Interacting Biomolecules with Enhanced Sampling*
13:45	Henrik Koch [862] *Generalized coupled cluster theory for ground state conical intersections*	Damien Laage [918] *On the mechanisms of hydronium and hydroxide diffusion in water*	Jan Halborg Jensen [440] *Computational discovery of new molecules that can actually be made*	Jian Liu [86] *Nonadiabatic Field: A Conceptually New Approach for Nonadiabatic Transition Dynamics*	Taye Demissie [673] *Computationally-Guided Design and Synthesis of Metal Complexes with Enhanced Cytotoxicity*
14:10	Karol Kowalski [199] *Coupled cluster downfolding formalisms for simulating many-body systems*	Jochen Blumberger [54] *Perturbed neural network potentials for condensed-phase simulations with external E-fields*	Kevin Naidoo [171] *An end-to-end integrated experimental computational drug discovery pipeline*	Peter Schürger [166] *Exact Factorization: New Perspective and Applications to Nonadiabatic Dynamics*	Petra Imhof [339] *INTERPLAY OF HYDRATION AND PROTON TRANSFER IN CYTOCHROME C OXIDASE*
14:25	Francesco Evangelista [348] *Reduced Dimensionality Models of Electrons via Exact Unitary Transformations*	Marco Nascimento [223] *Reducing the Coefficient of Friction of Water-Based Drilling Fluids.*	Gyula Hoffka [815] *Strategies for Generating Computationally Designed Enzymes with Nature-Like Efficiencies*	Oliver Kühn [412] *BSE@GW-Based Spin-Vibronic Quantum Dynamics Using the Linear Vibronic Coupling Model*	Ana Gamiz-Hernandez [917] *Proton coupled electron transfer in mycobacterial respiratory supercomplex III2IV2*
14:40	- 15:10	break			

Monday, June 23

	Session A4	Session B4	Session C4	Session D4	Session E4
	ELECTRONIC-STRUCTURE THEORY	MACHINE LEARNING	BIOSYSTEMS	CHEMICAL STRUCTURE & BONDING	QUANTUM DYNAMICS
	Explicit correlation	ML for chemical reactions	Macromolecules	Early elements	Ultrafast dynamics
	Chair: Wim Klopper	Chair: Sigbjørn Løland Bore	Chair: Qiang Cui	Chair: Gabriel Merino	Chair: Thomas Bondo Pedersen
15:10	Seiichiro Ten-no [874] *Simplified explicit correlation via projective transcorrelation*	Boris Kozinsky [971] *Symmetry and physics guided machine learning of microscopic interactions*	Modesto Orozco [819] *Nucleic acids in the frontier between AI and simulation.*	Miroslav Urban [270] *C—Li—C lithium bonds in metal cross-linked polyethylene chains*	Françoise Remacle [887] *Controlling ultrafast molecular reactivity with atto and few femtosecond pulses*
15:35	Ali Alavi [853] *Recent developments with Transcorrelated methods*	Fernanda Duarte [842] *Modelling Chemical Reactions in Solution with MLIPs*	Alessandra Magistrato [202] *Exploring RNA Metabolism through All-Atom Simulations*	ED Jemmis [163] *An Extended Rudolph Diagram explains the Structural Chemistry of Boron*	Michal Repisky [962] *Relativistic Real-Time Dynamics: Ultrafast Chirality in Molecules*
16:00	Éva Zsuzsanna Mihálka [470] *Geminal-based wavefunctions with an explicitly correlated extension*	Joakim Jestilä [246] *Data-efficient machine learning potentials for atomic layer deposition*	Mariastella Cascone [544] *Investigating the ET cascade in Cryptochrome 4 of different birds*	Celina Sikorska [738] *Boron-based superalkalis for inert molecules activation: a hybrid QM-QSPR approach*	H. Bernhard Schlegel [197] *Reducing the Cost of TD-CI Simulations of Strong Field Ionization*
16:15	Silvia Di Grande [587] *Pisa Composite Schemes: Advancing Scalable Accuracy in Thermochemical Predictions*	Jessica White [667] *Enhancing Mineral Carbonation Through Molecular Simulations on Mineral Surfaces*	David Carrasco De Busturia [165] *Multiphoton Absorption Spectra of Channelrhodopsin-2 via Multiscale Simulation Methods*	Tatiana Korona [276] *Defect-induced excited states in boron nitride - a theoretical study*	Jonathan Fetherolf [701] *Probing Nuclear–Electronic Orbital Dynamics with Cavity Emission*
16:30	- 17:00	break			

Monday, June 23

	Session A5	Session B5	Session C5	Session D5	Session E5
	ELECTRONIC-STRUCTURE THEORY	MACHINE LEARNING	COMPUTING & SOFTWARE	QUANTUM DYNAMICS	CATALYSIS & REACTIVITY
	Density-functional development	ML for chemical design	Quantum computing	Ultrafast dynamics	Electrochemistry and related
	Chair: Weitao Yang	Chair: David Balcells	Chair: Birgitta Whaley	Chair: Federica Agostini	Chair: Cristina Trujillo
17:00	Martin Head-Gordon [957] *Some recent advances in density functional theory*	Clémence Corminbœuf [446] *Do we really design molecules?*	Ivan Kassal [356] *Simulating Quantum Chemical Dynamics on Quantum Computers*	Fernando Martín García [663] *New directions in Theoretical Attosecond Chemistry*	Samira Siahrostami [21] *Computational Discovery of Materials for Selective Electrosynthesis of H2O2*
17:25	Erin Johnson [505] *Three short dispersion-corrected DFT vignettes*	Anatole von Lilienfeld [442] *Quantum machine learning in chemical space*	Marco Govoni [1007] *Simulating condensed systems on quantum computers using FCI-in-DFT embedding*	Ove Christiansen [959] *Time-dependent dynamics with vibrational coupled cluster theory*	Maria Besora [402] *Computational Studies of Polyoxometalate-Catalyzed Water Oxidation: Electrochemistry, Chemistry and Statistics*
17:50	Fritz Schaefer [687] *Does Jacob's Ladder Lead to Density Functional Heaven?*	Konstantinos Vogiatzis [10] *Molecular Topology Meets AI: Persistent Homology for Molecular Discovery*	Maria-Andreea Filip [419] *Current and Future Algorithms for Accelerated Hamiltonian Simulation*	Jiří Vaníček [691] *Can increasing the size of a molecule reduce decoherence?*	Tangui Le Bahers [169] *Using grand-canonical DFT to investigate electrochemical reactions on semiconductor surfaces*
18:30	Viktor Staroverov [154] *Electron-nucleus cusps without spherical averaging*	Thijs Stuyver [43] *Combining chemical theory and ML techniques to accelerate reaction discovery*	Yu Zhang [20] *Quantum Information-Inspired Algorithms for Quantum Chemistry*	Nazanin Jamshidi [140] *Quantum Dynamics of Plasmonic Nanocavities and Strong Coupling with Emitters*	Melissa Manetsch [362] *Quantifying and Tuning Local Electric Fields in Confined Catalytic Systems*
18:45	- 20:00	break			
20:00	- 22:00	Poster session 1			

Tuesday, June 24

	Session A1	Session B1	Session C1	Session D1	Session E1
	CATALYSIS & REACTIVITY	ELECTRONIC-STRUCTURE THEORY	BIOSYSTEMS	ELECTRONIC-STRUCTURE THEORY	SPECTROSCOPY
	Surfaces and heterogenous catalysis	Many-body methods & NCI	Bio/nanosystems	Relativistic quantum chemistry	Polarization models
	Chair: Stuart Macgregor	Chair: Seiichiro Ten-no	Chair: Michele Cascella	Chair: Trond Saue	Chair: Russell Boyd
08:30	Anastassia Alexandrova [38] *Catalytic interfaces in and out of equilibrium*	Katarzyna Pernal [875] *Two-fermion adiabatic connection methods for multireference electron correlation*	Daan Frenkel [703] *Multivalency and cell recognition*	Wenjian Liu [436] *Unified Implementation of Relativistic Hamiltonians and Wavefunctions*	Benjamin Stamm [798] *ddX: Polarizable Continuum Solvation from Small Molecules to Proteins*
08:55	Ataualpa Braga [901] *Cluster Modeling of Acid Sites and Catalytic Mechanisms in H-ZSM-5*	Janus Juul Eriksen [810] *Third-Generation Many-Body Expanded Full Configuration Interaction Theory*	Wataru Shinoda [782] *Endosomal Escape of Nucleic Acids via Lipid Nanoparticles: A Coarse-Grained Molecular Dynamics Study*	Jürgen Gauss [438] *Cholesky decomposition: relativistic quantum chemistry and magnetic properties*	Kaline Coutinho [938] *Solvent Effect in Electronic Properties: Approach with Solute&Solvent Polarization*
09:20	Mikhail Polynski [357] *Predicting Nanocatalyst Activity: Fast PES Exploration and Data-Efficient Machine Learning*	A. Daniel Boese [443] *Another Angle on Benchmarking Noncovalent Interactions*	Katie Wilson [97] *Modeling Bacterial Membranes: Role of Composition on Antimicrobial Peptide Mechanism*	Achintya Kumar Dutta [215] *Frozen-Natural-Spinors: An Efficient Framework for Relativistic Quantum Chemistry Methods*	Cedrix Dongmo Foumthuim [624] *Modeling Spectroscopic Properties of Biomolecules*
09:35	Basil Raju [47] *Novel Computational Approach for Determining Surface pKa at Metal-Aqueous Interfaces*	Andreas Hansen [121] *Accurate calculation of non-covalent interactions for large molecules*	João Coimbra [597] *The molecular mechanism of membrane disruption by venom PLA2-like proteins*	Erik Donovan Hedegård [497] *Treating heavy transition metals in solvation properly*	Tommaso Nottoli [305] *A Novel Implementation of CASSCF for Energy and Response Properties*
09:50	- 10:20	break			

Tuesday, June 24

	Session A2	Session B2	Session C2	Session D2	Session E2
	CATALYSIS & REACTIVITY Molecular and reaction design	ENERGY & MATERIALS Materials and energy	ELECTRONIC-STRUCTURE THEORY Berry phase & complex wave functions	QUANTUM DYNAMICS Ultrafast dynamics	BIOSYSTEMS Bio/nanosystems
	Chair: Odile Eisenstein	Chair: Leticia González	Chair: Henrik Koch	Chair: Fernando Martín García	Chair: Modesto Orozco
10:20	Satoshi Maeda [307] *Reaction pathway network representation for predicting unknown chemical reactions*	Laura Gagliardi [702] *Theory, Computation and Machine Intelligence for Reticular Chemistry*	Hardy Gross [949] *Molecular Berry phase without adiabatic approximation*	Federica Agostini [388] *Theory and simulations of ultrafast dynamics in molecules*	Biswarup Pathak [921] *Artificially Intelligent Nanopores for High-Throughput DNA Sequencing*
10:45	Markus Reiher [80] *Machine Learning for First-Principles Reaction Network Exploration*	Elena Besley [763] *Crystal embedded multi-reference method for studying strongly correlated materials*	Joseph Subotnik [686] *Beyond Born-Oppenheimer: Phase Space Approaches to Electronic Structure*	Morgane Vacher [820] *Simulating photo-induced processes in molecules: methodological aspects and attochemical applications*	Matteo Dal Peraro [728] *A "Structure Transformer" for Integrative Structural Biology and Molecular Design*
11:10	Derek Ahneman [161] *Building datasets and ML models to predict stepwise organic reactivity*	Tim Kowalczyk [239] *Electronically Excited States and Interlayer Heterogeneity in Covalent Organic Frameworks*	Ansgar Pausch [581] *Effects of the molecular Berry curvature in relativistic systems*	Yi Zhao [720] *Charge/Energy Transfer in Extended Systems Simulated from Stochastic Schrödinger Equations*	Gioacchino Schifino [580] *Computational Design of Aptasensors for West Nile Virus Detection*
11:25	GiovanniMaria Piccini [698] *Automatic Reaction Discovery by Biasing Deep-Learned Skewed Distributions*	Shubhajit Das [609] *Navigating the Landscape of Metal-Organic Framework Catalysts*	Bang Huynh [191] *Symmetry and interpretation of complex orbitals and wavefunctions*	Angela Wilson [680] *Quantum electron dynamics and polaritonic chemistry*	Samaneh Davoudi [79] *Understanding Estrogen's Affinity for GPER using Molecular Dynamics Simulations*
11:40	- 13:20	break			

Tuesday, June 24

	Session A3	Session B3	Session C3	Session D3	Session E3
	ELECTRONIC-STRUCTURE THEORY Density-functional development	MACHINE LEARNING ML for chemical reactions	MOLECULAR DYNAMICS Honorary session: 40 years of AIMD	QUANTUM DYNAMICS DMRG and MCTDH	CHEMICAL STRUCTURE & BONDING f-block elements
	Chair: Miroslav Urban	Chair: Francesco Paesani	Chair: Matteo Dal Peraro	Chair: Françoise Remacle	Chair: Pekka Pyykkö
13:20	Kieron Burke [922] *Approximate norms for approximate functionals*	Teresa Head-Gordon [847] *Machine Learning and Artificial Intelligence for Predictive Chemistry*	Roberto Car [987] *Ab-initio Molecular Dynamics of Ferroelectrics*	Irene Burghardt [666] *Multiconfigurational quantum dynamics of exciton transport in organic semiconductors*	Karin Fink [722] *Quantum-chemical calculations on magnetic and electronic properties of lanthanide compounds*
13:45	Eunji Sim [807] *Clarifying the Role of Density-Corrected DFT in Electronic Structure Calculations*	Dennis Salahub [91] *Towards ML- and QML-accelerated discovery of catalytic materials and mechanisms*	Ursula Röthlisberger [960] *Adaptive On-the-fly ML-MTS to Accelerate First-Principles Based Molecular Dynamics Simulations*	Zhigang Shuai [773] *Time-dependent DMRG simulation for spin transport in helical molecular wires*	Miho Hatanaka [713] *Theoretical and Data-Driven Approaches to Lanthanide Photofunctional Materials*
14:10	Jacques Desmarais [128] *Meta Generalized Gradient Approximation Made Magnetic*	Jordi Buils [479] *Data-Driven Methods for Solving Multi-Species Multi-Equilibria Self-Assembly of Metal-Oxide Nanoclusters*	Mark Tuckerman [395] *Beating the viscosity-conductivity inverse relation in emerging battery applications*	Yuki Kurashige [56] *Tensor and Neural networks for quantum dynamics with many degree-of-freedom*	Sergey Varganov [524] *Ab initio description of vibronic emission bands in lanthanide complexes*
14:25	Priya Priya [692] *Green's function formalism for kinetic energy density functional for atoms.*	Haobo Li [26] *Machine Learning Expands Computational Chemistry into Big Datasets for Catalysis*	Amin Alibakhshi [771] *Quantum Chemistry in Machine-Learning Era: How to Assess the Reliability?*	Henrik Larsson [134] *Rigorously computing thousands of vibrational states using tensor network methods*	Meagan Oakley [700] *Relativistic Quantum Chemical Investigation of Actinide Covalency Measured by EPR*
14:40	- 15:10	break			

Tuesday, June 24

	Session A4	Session B4	Session C4	Session D4	Session E4
	CATALYSIS & REACTIVITY	SPECTROSCOPY	BIOSYSTEMS	ELECTRONIC-STRUCTURE THEORY	ENERGY & MATERIALS
	Surfaces and heterogenous catalysis	Methods for excited electronic states	Multiscale modelling	Strong correlation & entanglement	Condensed systems
	Chair: Philippe Sautet	Chair: Frank Neese	Chair: Marco De Vivo	Chair: Piotr Piecuch	Chair: Marco Nascimento
15:10	Annabella Selloni [748] *Water dissociation at electrified oxide-electrolyte interfaces from machine learning simulations*	Emmanuel Fromager [755] *N-centered ensemble density functional theory of electronic excitations*	Benedetta Mennucci [832] *Photoinduced Biological Function: Bridging Electronic Excitations to the Functional Outcome*	Shuhua Li [881] *Block-correlated Coupled Cluster Methods for Strongly Correlated Systems*	Nicola Gaston [955] *Why is gallium liquid at room temperature?*
15:35	Akira Nakayama [681] *Molecular Insight into Adsorption and Conversion at the Liquid/Solid-Oxide Interface*	Weitao Yang [956] *ΔSCF Excited-State Approach: Theoretical Foundation, Fractional Charges, and Orbital Energies*	Paula Homem-de-Mello [685] *Design of Photosensitizers for Photodynamic Therapy*	Mario Piris [16] *Expanding the Frontiers of Natural Orbital Functional Theory*	Pavel Jungwirth [664] *Electrolyte-to-metal transition in ammonia solutions of alkali metals by AIMD*
16:00	Seungjae Kwak [437] *Muti-scale Approach to Understanding Superlattice Area Selective Atomic Layer Deposition*	Momir Mališ [787] *Improving the ΔSCF method for excited electronic states*	Yingjie Wang [117] *Multiscale Regulation of Light-Harvesting and Quenching in LHCII protein*	Jiří Pittner [77] *Spin-free orbital entropy, mutual information, and entanglement analysis*	Sheh-Yi Sheu [19] *High-Performance Energy-Free Desalination*
16:15	Francesc Viñes Solana [89] *Computational Assessment of MXenes Bandgap Engineering for Photocatalytic Water Splitting*	Lars Goerigk [139] *Time-dependent range-separated double-hybrids with spin scaling for difficult excited-state problems*	Sebastian Reiter [594] *Multiscale Modeling of Photosystem I Light-Harvesting in Diverse Environments*	Sarai Dery Folkestad [94] *Towards spin completeness with entanglement CCSD for doublet systems*	Jun-Ho Choi [50] *Molecular aggregation and microheterogeneity in osmolyte solutions*
16:30	- 17:00	break			

Tuesday, June 24

	Session A5	Session B5	Session C5	Session D5	Session E5
	BIOSYSTEMS Cheminformatics & medicinal chemistry	ELECTRONIC-STRUCTURE THEORY Methods for larger systems	CATALYSIS & REACTIVITY Reactants, reactions, and catalysis	SPECTROSCOPY Circular dichroism	EXOTIC SYSTEMS Strong fields and high pressure
	Chair: Ursula Röthlisberger	Chair: David Sherrill	Chair: Annia Galano	Chair: Kenneth Ruud	Chair: Peter Schwerdtfeger
17:00	William Jorgensen [808] *Impact of Free Energy Calculations for Chemistry and Drug Discovery*	Christian Ochsenfeld [952] *Efficient quantum-chemical methods for excited states, properties, and reaction networks*	David Wales [969] *Energy landscapes: from molecules to machine learning*	Daniel Crawford [757] *Advanced Quantum Chemical Methods for Chiroptical Spectroscopy*	Stella Stopkowicz [941] *Predicition and Assignment of Strongly Magnetized White Dwarf Spectra*
17:25	Zoe Cournia [981] *Predicting protein-ligand, protein-protein, protein-membrane interactions using molecular simulations and AI*	Hiromi Nakai [723] *Breaking Barriers in Fragmentation Methods for Long-Range Interactions*	Feliu Maseras [674] *Beyond free energy profiles: microkinetic models*	Luuk Visscher [814] *Modelling electronically enhanced vibrational circular dichroism spectra: challenges and solutions*	Andrew Wibowo-Teale [671] *Molecular Aharonov–Bohm-type interferometers based on porphyrin nanorings*
17:50	Stacey Wetmore [321] *A Multipronged Computational Investigation of the Chemistry of Modified RNA*	Filippo Lipparini [826] *CCSD energies and structures for larger, symmetric molecules*	Sebastian Kozuch [2] *Tunneling of Molecules: the Weirdest Side of Chemical Reactivity*	WanZhen Liang [243] *Modeling the Photophysical Processes of Organic Molecular Aggregates*	Eva Zurek [697] *Unusual Chemistry and New States of Matter at Extreme Pressures*
18:30	Christoph Riplinger [714] *Deciphering Ligand Interactions with Biomolecules Using Quantum Mechanical Methods*	Maristella Alessio [187] *Coupled-Cluster Treatment of Large and Complex Open-Shell Systems*	Masataka Nagaoka [44] *Molecular Simulation of Complex Reaction Systems: The Red Moon Approach*	Marco Caricato [138] *Optical and Chiroptical Linear Response Properties of Materials*	Mercedes Alonso [393] *Modeling Atomic and Molecular Behavior under Isotropic Pressure*
18:45	- 20:00	break			
20:00	- 22:00	Poster session 2			

Wednesday, June 25

Plenary P3

Chair: Peter Gill

08:30 Gustavo Scuseria [848]
Symmetry-Projected Coupled Cluster Theory

09:10 Katharina Boguslawski [879]
Is simpler better? Alternative wave function approaches for molecular modeling

09:50 - 10:20 break

Plenary P4

Chair: Martin Head-Gordon

10:20 Luhua Lai [851]
Computational approaches for making undruggable targets druggable

11:00 Heather Kulik [418]
What has machine learning taught us about transition metal chemistry?

11:40 excursion

20:00 Congress dinner

Thursday, June 26

	Session A1	Session B1	Session C1	Session D1	Session E1
	ELECTRONIC-STRUCTURE THEORY	SPECTROSCOPY	BIOSYSTEMS	CHEMICAL STRUCTURE & BONDING	ENERGY & MATERIALS
	Methods for periodic systems	Methods for excited states	Multiscale modelling	Analysis	Photophysics and photochemistry
	Chair: Christian Ochsenfeld	Chair: Emmanuel Fromager	Chair: Stefano Vanni	Chair: Henry Rzepa	Chair: Zhigang Shuai
08:30	Georg Kresse [831] *Machine learning and beyond DFT methods: enabling materials modelling*	Julia Westermayr [364] *Machine Learning for Excited States*	Qiang Cui [689] *Recent developments and applications of QM/MM-ML methods*	Matthias Bickelhaupt [670] *Paradigm Shifts in Chemical Theory*	Dage Sundholm [797] *Optical and photophysical properties of fifth generation light-emitting molecules*
08:55	Lin Lin [571] *Finite-size error in quantum chemistry methods for periodic systems*	Hannes Jónsson [660] *Rydberg/charge-transfer excited states using saddle point searches and neural-network CI*	Garnet Chan [872] *Towards discovering reactivity with QM methods in biological systems*	Frank de Proft [813] *Conceptual Density Functional Theory Based Reactivity Indices: Analytical Evaluation*	Jing Ma [888] *Machine Learning of NRR and CO2RR Reaction Activities and Selectivities*
09:20	David Tew [870] *DLPNO-MP2 for Periodic Systems in the Turbomole Program*	Thomas Froitzheim [81] *Δg-xTB: Excited states with state-specific extended Tight-Binding*	Andrea Pérez-Villa [504] *Synergistic Integration of Co-Folding and QM/MM calculations for Protein-Ligand Binding*	Inbal Tuvi-Arad [749] *Exploring Hidden Structural Insights with Continuous Symmetry and Chirality Measures*	Dana Nachtigallová [636] *Tuning On-Surface Photoactivity: The Role of π-Conjugation in Anhydride-Functionalized Molecules*
09:35	Philip Hoggan [13] *Quantum Monte Carlo resolving metal catalyst activation barriers: Hydrogen production..*	Elli Selenius [790] *Orbital-optimized density functional calculations of challenging charge transfer excitations*	Andrea Levy [601] *Atom-centered electric multipole moments dynamically generated from QM/MM MD simulations*	Jacob Toney [394] *Graph neural networks predicting metal-ligand coordination in transition metal complexes*	Sofia Canola [582] *Molecules meet light in STM: atomically-resolved visualization of light-mediated processes*
09:50	- 10:20	break			

Thursday, June 26

	Session A2	Session B2	Session C2	Session D2	Session E2
	ELECTRONIC-STRUCTURE THEORY	CATALYSIS & REACTIVITY	BIOSYSTEMS	ENERGY & MATERIALS	COMPUTING & SOFTWARE
	Simpler model systems	Reactants, reactions, and catalysis	Multiscale modelling	Photophysics and photochemistry	Software
	Chair: Anna Krylov	Chair: Manuel Yañez	Chair: Garnet Chan	Chair: Dage Sundholm	Chair: Daniel Crawford
10:20	Stefan Grimme [825] *Status report on the new g-xTB tight-binding method*	Evert Jan Meijer [943] *Elucidating the Role of Solvent and Cations in CO2 Conversion*	Carme Rovira [863] *Deciphering Carbohydrate-Active Enzymes: Reactions, Conformations, and Mechanisms*	Kumar Vanka [899] *Understanding the Behaviour of Unidirectional Molecular Motors with Computational Chemistry*	Patrick Norman [898] *VeloxChem: Science and education-enabling platform for quantum molecular modeling*
10:45	Peter Schwerdtfeger [92] *100 years of Lennard-Jones potentials: Applications to the solid state*	Bastian Skjelstad [715] *Wacker oxidation insights from density-functional theory and machine-learned interatomic potentials*	Marco De Vivo [817] *Targeting RNA at the Conserved Active Site of Splicing Machinery*	Leticia González [964] *Unravelling reaction pathways in photoswitchable molecules*	Susi Lehtola [799] *Progress towards a reusable software stack in quantum chemistry*
11:10	Per Siegbahn [212] *Why is DFT so much better for larger systems ?*	Amalia Poblador Bahamonde [880] *Sulfinyl-tethered N-heterocyclic carbene ligands: structure and reactivity by computational approach*	Stefano Serapian [120] *Multiscale modelling of allostery in proteins*	Enrico Tapavicza [523] *Photodynamics and chemical compound space of light-driven molecular nanomotors*	John Herbert [24] *Open-Source Framework for Fragment-Based Quantum Chemistry*
11:25	Itai Panas [679] *Electron Correlation Corrected Hartree-Fock Theory - Back to the Future*	Zhexuan Song [654] *Deciphering the Acceleration Mechanisms of Simple Organic Reactions in Microdroplets*	Allison Keys [226] *CH–π Interactions Confer Orientational Flexibility in Protein-Carbohydrate Binding Sites*	Enrique Manuel Arpa [411] *Exploiting excited-state aromaticity to enhance photochemical organic reactivity*	Alexander Stark [157] *Improving Slater Orbital Integration Accuracy through Prolate Spheroidal Coordinates*
11:40	- 13:20	break			

Thursday, June 26

	Session A3	Session B3	Session C3	Session D3	Session E3
	ELECTRONIC-STRUCTURE THEORY	CATALYSIS & REACTIVITY	MACHINE LEARNING	SPECTROSCOPY	TEACHING & EDUCATION
	Density-functional development	Molecular and reaction design	ML for simulations	Rotovibrational spectra	Teaching & education
	Chair: Jiali Gao	Chair: Ainara Nova	Chair: Konstantinos Vogiatzis	Chair: Sonia Coriani	Chair: Trygve Helgaker
13:20	Stefan Vučković [837] *Bridging Traditional Methods and Machine Learning in Density Functional Developments*	Annia Galano [508] *CADMA-Chem: A Computational Protocol to Design Multifunctional Antioxidants*	Yi Luo [737] *Autogeneration of functional molecule structures from spectroscopies with machine learning*	Attila Császár [931] *MARVEL and SNAPS*	Anders Malthe-Sørenssen [998] *Computational literacy as a driver for disciplinary renewal in chemistry*
13:45	Martin Kaupp [661] *Beyond-zero-sum-game density functionals based on the exact-exchange energy density*	Vidar Jensen [946] *Automated de Novo Design of Transition-Metal Catalysts*	Yi Qin Gao [882] *AI assisted molecular modeling and simulations*	Guntram Rauhut [106] *Toward a convenient calculation of rovibrational spectra*	Peter Taylor [1001] *The "royal road" to expertise in quantum chemistry*
14:10	Hans Jørgen Aa. Jensen [457] *Variational MC-srPDFT – a multiconfigurational short-range on-top pair-density model*	Cristina Trujillo [36] *Computationally Led Catalyst Design*	Amanda Arcidiacono [537] *Understanding excited states of carotenoids in environments with machine learning*	Ayaki Sunaga [735] *Variational Vibrational States of Methanol (12D)*	Dirk Andrae [367] *Simple(r), yet (more) efficient maths teaching for students of chemistry*
14:25	Aaron Garrison [159] *Machine Learning Prediction of Optimal Exchange Fractions in Hybrid Functionals*	Wataru Matsuoka [237] *Virtual Ligand Assisted-Optimization: A Rational Strategy for Ligand Engineering*	Krzysztof Szalewicz [730] *New life for "classical" force fields in machine-learning age*	Frederik Tielens [72] *Theoretical Raman Spectroscopy in Industry: From Computational Modeling to Applications*	Henry Rzepa [12] *From FAIRSpec data and Finding aids to a FAIRComp specification.*
14:40	- 15:10	break			

Thursday, June 26

	Session A4	Session B4	Session C4	Session D4	Session E4
	CATALYSIS & REACTIVITY	ENERGY & MATERIALS	ELECTRONIC-STRUCTURE THEORY	MACHINE LEARNING	SPECTROSCOPY
	Reactants, reactions, and catalysis	Materials and energy	Optimization in quantum chemistry	ML for electronic structure	Positrons & weak interactions
	Chair: Feliu Maseras	Chair: Evert Jan Meijer	Chair: Erik Tellgren	Chair: Hiromi Nakai	Chair: Edit Mátyus
15:10	Jin Wen [800] *Machine Learning-Enhanced Ultrafast Dynamics in Complex Systems: Methods and Applications*	Debra Bernhardt [751] *Ionic conductivity and fluid flow: predictions from response theory*	Éric Cances [742] *Optimization problems in electronic structure calculation*	Paola Gori-Giorgi [867] *Machine Learning and Electronic Structure Theory*	Gustavo Aucar [861] *On molecular chirality and weak forces, entanglement and NMR-J couplings*
15:35	Fahmi Himo [928] *Modeling Reactions in Supramolecular Systems*	Sara Bonella [827] *Classical simulations of interfaces in supercapacitors*	Roland Lindh [672] *The Reduced Variation Optimization Procedure: A qualitative analysis*	Matthias Kick [233] *Super-Resolution Methods for Accelerating Large-Scale Electronic Structure Calculations*	Robert Berger [360] *Models, predictions of parity-violating level shifts in small chiral molecules*
16:00	Johannes Hoja [575] *Towards Kinetics of Molecular Crystals: Polymorph Transitions and Chemical Reactions*	Virginia Carnevali [538] *Nanoscale effects in α-FAPbI3 evinced by large-scale ab initio simulations*	Giovanni Scalmani [619] *Stability, CIS/TDA, and TD for complex and general HF/KS-SCF*	Angel Martín Pendás [58] *Chemical Machine Learning with Real-Space Descriptors*	Dermot Green [256] *Many-body theory of positron interactions with atoms and polyatomic molecules*
16:15	Michele Assante [769] *Combined DFT and ML modelling for metallaphotoredox sp2-sp3 cross-coupling reactions.*	Tuanan C. Lourenço [334] *Multiscale Investigation of Ionic Liquid-based Electrolytes for Sodium-ion Batteries*	Hugh Burton [712] *Restricted open-shell SCF theory for low-spin coupling*	Tomáš Bučko [214] *Benchmarking electronic structure methods in anharmonic finite-temperature thermodynamic calculations*	Kenneth Jordan [1] *Diffusion Monte Carlo Calculations of Positron Affinities*
16:30	- 17:00	break			

Thursday, June 26

	Session A5	Session B5	Session C5	Session D5	Session E5
	SPECTROSCOPY	ELECTRONIC-STRUCTURE THEORY	ENERGY & MATERIALS	BIOSYSTEMS	CHEMICAL STRUCTURE & BONDING
	Spectroscopy & energy surfaces	Beyond standard DFT	Materials and energy	Bio/nanosystems	Coordination chemistry
	Chair: Abril Castro	Chair: Paola Gori-Giorgi	Chair: Laura Gagliardi	Chair: Carme Rovira	Chair: ED Jemmis
17:00	Sonia Coriani [925] *Modeling Spectroscopic Observables on Classic and Hybrid-Quantum Computers*	Paul Ayers [733] *The 1-electron Reduced Density Matrix Functional: An Optimal Transport Approach*	Marie-Liesse Doublet [966] *Materials for Energy Storage : Challenges and Related Issues*	Sergio Pantano [417] *Stripping off a naked virus: Modeling the Cirocvirus genome.*	Gabriel Merino [392] *Recent Advances in Planar Hypercoordinate Atom Chemistry*
17:25	Anna Krylov [382] *Probing complex potential energy surfaces of metastable states by spectroscopy*	Jiali Gao [904] *Multistate Density Functional Theory and MultiState Energy Decomposition Analysis (MS-EDA)*	Emi Minamitani [93] *Persistent homology elucidates structure-properties relationships in amorphous solids*	Cristiana Di Valentin [794] *Modeling complex nanosystems for drug delivery, targeted therapy and imaging*	Jeanet Conradie [118] *DFT methods and techniques for identifying Jahn-Teller isomers of manganese(III)-complexes*
17:50	Ida-Marie Høyvik [721] *Charge localized electronic wave functions for ground and excited states*	Andreas Görling [220] *Optimized-effective-potential method for accurate TDDFT excitation energies with standard density-functionals*	Gloria I. Cárdenas-Jirón [795] *Charge Transport of Dyes and Electrodes by Molecular Junction Modeling*	Stefano Vanni [643] *Good fat or bad fat? From forcefield development to physiology*	Julien Panetier [53] *Computational Modeling of CO Dehydrogenase Model Systems for CO2 Fixation*
18:30	Takeshi Sato [651] *Electronic structure and dynamics simulations with classical and quantum computers*	Lucien Dupuy [631] *KS-DFT Beyond Born-Oppenheimer: Exact Mapping to an Electronically Non-Interacting Molecule*	Antti Karttunen [607] *Pyroelectricity of Ferroelectric BaTiO3 and PbTiO3 from Density Functional Theory*	Maurício Coutinho Neto [732] *Coarse Grain SAXS Modeling of Lipopeptide Self-Assembled Structures*	Konrad Patkowski [122] *Influence of three-body interactions on halogen bonding*
18:45	- 20:00	break			
20:00	- 22:00	Poster session 3			

Friday, June 26

Plenary P5

Chair: Peter Gill

08:30 Mario Motta [983]
Quantum chemistry calculations using classical and quantum computers in concert

09:10 Edit Mátyus [934]
Molecular quantum dynamics by solving the rovibrational Schrödinger equation

09:50 - 10:20 break

Plenary P6

Chair: Peter Gill

10:20 Alexander Sokolov [415]
Efficient multireference methods for excited states and spectroscopy

11:00 Thomas Jagau [939]
Recent progress in complex-energy electronic-structure methods

11:40 Closing remarks